

# **DRAFT FINAL REPORT**

## **Intermedia Transfer Factors for Contaminants Found at Hazardous Waste Sites**

### **BENZENE**

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Prepared for:

The Office of Scientific Affairs  
The Department of Toxic Substances Control (DTSC)  
and the California Environmental Protection Agency  
in Support of the CalTOX Model

December 1994

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## FORWARD

The Department of Toxic Substances Control (DTSC), within the California Environmental Protection Agency, has the responsibility for managing the State's hazardous-waste program to protect public health and the environment. The Office of Scientific Affairs (OSA) within the DTSC provides scientific assistance in the areas of toxicology, risk, environmental assessment, training, and guidance to the regional offices within DTSC. Part of this assistance and guidance is the preparation of regulations, scientific standards, guidance documents, and recommended procedures for use by regional staff, local governmental agencies, or responsible parties and their contractors in the characterization and mitigation of hazardous-waste-substances-release sites. The CalTOX model has been developed as a spreadsheet model to assist in exposure and health-risk assessments that address contaminated soils and the contamination of adjacent air, surface water, sediments, and ground water.

The modeling effort includes multimedia transport and transformation models, exposure scenario models, and efforts to quantify and reduce uncertainty in multimedia, multiple-pathway exposure models. Use of the CalTOX model requires that we determine the intermedia transfer factors (ITFs) that define concentration relationships between an exposure medium and the environmental medium that is the source of the contaminant. ITFs are chemical and physical parameters which serve as inputs in the CalTOX model analysis.

This report provides a set of ITFs needed to run the CalTOX model for benzene. For this chemical, we have conducted a critical review of existing literature for measured values and estimation methods in order to compute an arithmetic mean ( $\bar{x}$ ), a coefficient of variation (CV), and plausible range for each ITF.

## OVERVIEW

The purpose of this report is to provide a set of chemical-specific intermedia-transfer factors (ITFs) for benzene. We have carried out a critical review of the existing literature in order to identify a mean value, coefficient of variation (CV) and value range for the ITFs listed in Table 1. For values used to define a given parameter, our highest priority was given to experimental values reported in the primary scientific literature, that is, peer-reviewed journals. For parameters that are not readily available from the primary literature, widely cited secondary references such as Lyman et al. (1982, 1990), Verschueren (1984), Howard et al. (1990, 1991), Mackay et al. (1992), the CRC Handbook (1989-90) and the Merck Index (1983, 1989) are used to establish parameter values. When measured values are not available from either the primary literature or secondary references, estimates of ITF parameter values are based on estimation equations that are available in the primary literature. Typically, these estimation methods relate ITFs to other measured contaminant parameters using quantitative-structure-activity-relationship (QSAR) methods. In these cases, parameter values estimated from a QSAR method are treated as the arithmetic mean and the estimation error of the method is used to determine the CV. Table 1 summarizes the units required by the CalTOX model, the values of chemical specific physico-chemical properties, distribution coefficients, biotransfer and bioconcentration factors, and transformation half-lives obtained in this study.

### CalTOX Chemical-Specific Input Requirements

The CalTOX model uses three sets of input data—one describing the chemical-specific properties of the contaminants, a second providing properties of the environment or landscape receiving the contaminants, and a third that defines for exposure assessment the characteristics of individuals in various age/sex categories and the characteristics of the micro-environments in which they live or from which they obtain water and food. Each of the inputs in these sets must be described in terms of a mean value with an estimated coefficient of variation, which describes the uncertainty or variability associated with that parameter. This report addresses mean value, CV, and range of values needed to characterize chemical-specific inputs.

#### *Physicochemical Properties*

Physicochemical properties include molecular weight, octanol-water partition coefficient, melting point, vapor pressure, Henry's law constant, diffusion coefficients in air and water, and the organic-carbon partition coefficient. The octanol-water partition coefficient provides a measure of the extent of chemical partitioning between water and octanol at equilibrium and is used as a basis for estimating other ITF parameters. The melting point is the temperature at which a compound makes the transition from a solid to a liquid phase. Vapor pressure is the pressure exerted by a chemical vapor in equilibrium with its solid or liquid phase. Water solubility is the upper limit on a chemical's dissolved concentration in pure water, at a specified temperature.

**Table 1. Summary of Chemical Properties for Benzene**

Description	Symbol <sup>a</sup>	Mean Value	Coefficient of Variation	Number of Values
Molecular Weight (g/mol) $\times 10^{-5}$	MW	78.11	$1.7 \times 10^{-5}$	5
Octanol-Water Partition Coefficient	K <sub>ow</sub>	150	0.24	12
Melting Point (K)	T <sub>m</sub>	278.6	$2.5 \times 10^{-4}$	1
Vapor Pressure (Pa)	VP	12700	0.036	6
Solubility (mol/m <sup>3</sup> )	S	22	0.059	21
Henry's Law Constant (Pa-m <sup>3</sup> /mol)	H -	570	0.16	7
Diffusion Coefficient in Pure Air (m <sup>2</sup> /d)	D <sub>air</sub>	0.76	0.08	e
Diffusion Coefficient in Pure Water (m <sup>2</sup> /d)	D <sub>water</sub>	$9.6 \times 10^{-5}$	0.25	e
Organic Carbon Partition Coefficient	K <sub>oc</sub> -	55	0.57	17
Distribution Coefficient in Ground-Surface and Root-Zone Soil	K <sub>d_s</sub> -	b	e	e
Distribution Coefficient in Vadose-Zone Soil	K <sub>d_v</sub> -	b	e	e
Distribution Coefficient in the Ground-Water Zone	K <sub>d_q</sub> -	b	e	e
Distribution Coefficient in Ground Water Sediment	K <sub>d_d</sub> -	b	e	e
Partition Coefficient in Plants Relative to Soil Concentration [ppm (pFM)/ppm (sFM)]	K <sub>ps</sub> -	3.0	0.38	2
Biotransfer Factor in Plants Relative to Contaminant Air Concentration (m <sup>3</sup> [a]/kg[pFM])	K <sub>pa</sub> -	0.0087	14	e
Biotransfer Factor in Milk Relative to Cattle-Diet Contaminant Intake (d/kg)	B <sub>k</sub> -	$1.6 \times 10^{-6}$	11	e
Biotransfer Factor in Meat Relative to Cattle-Diet Contaminant Intake (d/kg)	B <sub>t</sub> -	$1.6 \times 10^{-5}$	13	e
Biotransfer Factor in Eggs Relative to Hen-Diet Contaminant Intake (d/kg)	B <sub>e</sub> -	0.0012	14	e
Biotransfer in Breast Milk Relative to Contaminant Intake by the Mother (d/kg)	B <sub>bm</sub> k -	$3.0 \times 10^{-5}$	10	e
Bioconcentration Factor in Fish Relative to Contaminant Water Concentration	BCF -	6.8	0.43	3
Skin Permeability Coefficient (cm/h)	K <sub>p_w</sub> -	0.19	0.57	2
Skin-Water/Soil Partition Coefficient	K <sub>m</sub> -	15	1.4	2
Reaction Half-Life in Air (d)	T <sub>half_a</sub>	5.9	0.51	12
Reaction Half-Life in Ground-Surface Soil (d)	T <sub>half_g</sub>	190	1.5	2
Reaction Half-Life in Root-Zone Soil (d)	T <sub>half_s</sub>	190	1.5	2
Reaction Half-Life in the Vadose-Zone Soil (d)	T <sub>half_v</sub>	240	1.3	5
Reaction Half-Life in Ground-Water Zone Soil (d)	T <sub>half_q</sub>	240	1.3	5
Reaction Half-Life in Surface Water (d)	T <sub>half_w</sub>	11	0.51	6
Reaction Half-Life in the Sediment (d)	T <sub>half_d</sub>	220	1.4	5

<sup>a</sup>Values followed by a "-" include default equations that can be used for estimations

<sup>b</sup>K<sub>d</sub> = [(K<sub>oc</sub>)  $\times$  (fraction organic matter)], a site and soil zone specific parameter

<sup>e</sup>estimated parameter value



Henry's law constant is a measure at equilibrium of the ratio of chemical activity in the gas above a liquid to chemical activity in the liquid. Diffusion coefficients describe the movement of a molecule in a liquid or gas medium as a result of differences in concentration within the medium. They are used to calculate the dispersive component of chemical transport. The higher the diffusion coefficient, the more likely a chemical is to move in response to concentration gradients. The organic-carbon partition coefficient provides a measure of chemical partitioning between organic carbon (in soils, rocks, and sediments) and water. The higher the  $K_{OC}$ , the more likely a chemical is to bind to the solid phase of soil or sediment than to the liquid phase.

#### *The Solid-Water Distribution Coefficients*

The distribution or sorption coefficient,  $K_d$ , is the concentration ratio, at equilibrium, of chemical attached to solids and/or particles (mol/kg) to chemical concentration in the solution, mol/L. When  $K_{OC}$  is multiplied by the fraction organic carbon in a soil or sediment, we obtain an estimate of the soil/water or sediment/water partition coefficient. CalTOX requires, as input, distribution coefficients for ground-surface, root-zone, and vadose-zone soil; ground-water-zone rock or soil, and surface-water sediments.

#### *Biotransfer Factors and Bioconcentration Factors*

The CalTOX model requires, as input, general relationships that can be used to estimate partition coefficients between air and plants; between soil and plants; between animal feed intake and animal-based food products; between surface water and fish; between the human mother's uptake and breast milk; between skin and water; and between skin uptake and concentration in skin water.

The chemical-specific plant-air partition coefficient,  $K_{pa}$ , represents the ratio of contaminant concentration in above-ground plant parts, in mg/kg (fresh mass), to contaminant concentration in the gas-phase of the atmosphere mg/m<sup>3</sup> (air). The plant-soil partition coefficient,  $K_{ps}$ , expresses the ratio of contaminant concentration in plant parts, both pasture and food, in mg/kg (plant fresh mass) to concentration in wet root-zone soil, in mg/kg.

The biotransfer factors  $B_t$ ,  $B_k$  and  $B_e$  are the steady-state contaminant concentrations in, respectively, fresh meat, milk, and eggs; divided by the animals' daily contaminant intake. These factors are expressed in units of (mg/kg)/(mg/d), or kg/d. Unlike bioconcentration factors, which express steady-state concentration ratios between animal tissue and a specific environmental medium, biotransfer factors express the steady-state relationship between intake and tissue or food-product concentrations.

Lactating women can transfer to breast milk their intake of contaminants from all intake routes—ingestion, inhalation, and dermal contact.  $B_{bmk}$  is the biotransfer factor for milk-concentration versus the mother's intake. This relationship may also be

described as the ratio of contaminant concentration in mother's milk divided by the mother's daily intake of that contaminant, in units of d/kg (milk).

The bioconcentration factor BCF provides a measure of chemical partitioning between fish tissue based on chemical concentration in water.

Chemical specific exposure factors used in CalTOX include the skin-water and skin-soil partition coefficients.  $K_m$  is the skin-water partition coefficient in  $\text{cm}^3$  (water)/ $\text{cm}^3$  (skin). In order to estimate the skin-soil partition factor,  $K_m^{\text{soil}}$ , with units  $\text{cm}^3(\text{soil})/\text{cm}^3(\text{skin})$ , we divide equation  $K_m$  by the sorption coefficient  $K_d$  for soil, or

$$K_m^{\text{soil}} = \frac{K_m}{K_d}$$

$K_{p\_w}$  is the steady-state permeability coefficient in cm/hour for a contaminant from water on skin through stratum corneum and can either be based on a measured value or estimated values.

#### *Chemical-Specific Transformation Process Half-Lives*

Chemical transformations, which may occur as a result of biotic or abiotic processes, can have a profound effect on the persistence of contaminants in the environment. Experimental methods and estimation methods are available for defining these fate processes in a variety of media. Specific information on the rates and pathways of transformation for individual chemicals of concern should be obtained directly from experimental determinations, if possible, or derived indirectly from information on chemicals that are structurally similar. CalTOX makes use of media- and reaction-specific reaction half-lives to establish rate constants for transformation removal processes that include photolysis, hydrolysis, oxidation/reduction, and microbial degradation.

Transformation-rate half-lives are among the more uncertain parameters in the CalTOX model. There are typically few available measurements or ranges of estimated values in the primary and secondary literature. Most of the available half-life values are obtained from limited measurements for environmental media that are not necessarily representative of those in California. These values often involve scientific judgment as much as measurement. In making use of these data, we expanded the range of the reported values by a factor of 5 when only 2 or 3 representative values are presented and by a factor of 10 when only one value is provided. If 4 or more measured values are available, these uncertainty factors are not applied. In order to express the lack of reliability associated with a limited number of measured values for a parameter, these uncertainty factors are used to express both large uncertainty and significant variability.

## Statistical Methods

Each of the inputs to CalTOX must be described by a mean value and an estimated coefficient of variation which describes the uncertainty or variability associated with that parameter. For input values that are derived from a number of measured values, the mean and coefficient of variation are obtained from the arithmetic mean and the arithmetic standard deviation of the inputs. For estimated input values, the mean and coefficient of variation are obtained from an estimation equation and the residual error of the estimation equation. The methods we used to obtain these values are described here.

### *Mean and Coefficient of Variation*

The arithmetic mean ( $\bar{x}$ ) is used to represent all inputs that are derived from a number of measured values—even those that might have geometric distributions. The ( $\bar{x}$ ) is computed by summing the reported values and dividing this sum by the total number of observations:

$$\text{Arithmetic mean } (\bar{x}) = \frac{\sum_{i=1}^n x_i}{n} \quad (\text{Eqn. 1})$$

Where  $\sum_{i=1}^n x_i$  is the sum of the observed values and  $n$  is the number of observations. In this case, the coefficient of variation (CV) is computed by dividing the arithmetic standard deviation ( $S_n$ ) by the mean. Standard deviation and CV are computed according to the following equations:

$$\text{standard deviation } (S_n) = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n}} \quad (\text{Eqn. 2})$$

$$\text{coefficient of variation (CV)} = \frac{S_n}{\bar{x}} \quad (\text{Eqn. 3})$$

It should be noted that, based on the central limit theorem of statistics, the confidence associated with the estimate of  $\bar{x}$  from above becomes large as the number of samples used to estimate  $\bar{x}$  also becomes large. Therefore, the reliability of the estimates of *mean* and *CV* of a parameter are low when the sample size is small. It is beyond the scope of this document to explicitly address the reliability of these estimates. Nonetheless, in order to give an indication of potential reliability problems, we list the number of measurements used to estimate the mean and CV of each parameter in the last column of Table 1.

### *Estimation Equations and the Residual Errors of the Estimation Method*

Estimates of some CalTOX inputs are based on regression equations that relate a parameter value to some measure of structure or activity associated with the contaminant. These methods are referred to as quantitative structure-activity relationship (QSAR) methods. The reliability of a parameter-value estimated in this way is defined by the precision of these QSAR methods.

Our estimate of precision in QSAR estimation methods is based on calculating,  $S_e$ , the *standard error of the estimate* (or standard deviation of the residuals). This error calculation is based on the regression equations and fragment models used to derive a parameter value. To illustrate, when the value of parameter such as the organic-carbon partition coefficient ( $K_{oc}$ ) is estimated using a regression or correlation analysis, the  $S_e$  is calculated using the following approach (Hamburg, 1970). First, since it is typical that it is the  $\log K_{oc}$  (not  $K_{oc}$  itself) that is estimated from a regression equation, we calculate the  $S_e$  of  $\log K_{oc}$  according to

$$S_e \text{ of } \log K_{oc}^{est} = \sqrt{\frac{\sum_{i=1}^n (\log K_{oc}^{msd} - \log K_{oc}^{est})^2}{(n-2)}} \quad (\text{Eqn. 4})$$

where  $n$  is the number of chemicals used in the estimation protocol and  $K_{oc}^{est}$  refers to the estimated property ( $K_{oc}$  in this case) and  $K_{oc}^{msd}$  refers to the corresponding measured values used to carry out the regression. In order to calculate the  $S_e$  of  $K_{oc}$  we make use of the transformation

$$GSD(K_{oc}^{est}) = 10^{(S_e \text{ of } \log K_{oc}^{est})} \quad (\text{Eqn. 5})$$

to calculate the geometric standard deviation of  $S_e$  (GSD) of  $K_{oc}^{est}$ , which is simply the GSD of the  $K_{oc}$  estimate, that is  $GSD(K_{oc}^{est})$ . It has been shown by Atchison and Brown (1957) that the relationships between the GSD and CV for log normal distributions are as follows

$$GSD = \exp\{\sqrt{\ln(1+CV^2)}\} \quad (\text{Eqn. 6})$$

$$CV = \sqrt{\left(\exp\{[\ln(GSD)]^2\} - 1\right)} \quad (\text{Eqn. 7})$$

Since the implicit assumption of a regression for estimating the log of  $K_{oc}$  is that any estimated value,  $\log(K_{oc}^{est})$ , is centered on normal distribution with standard deviation equal to  $S_e$  of  $\log K_{oc}$  it follows that the corresponding estimated value of  $K_{oc}$  is centered on a log normal distribution with GSD ( $K_{oc}^{est}$ ) and with

$$CV(K_{oc}^{est}) = \sqrt{\exp\{[\ln(GSD(K_{oc}^{est}))]^2\} - 1} \quad (\text{Eqn. 8})$$

This approach is used to estimate CVs for the estimation equations presented in this document.

In some cases the error term, CV for example, is calculated by combining through the operations of multiplication and division the CVs of two or more parameters. For example the CV in the ration  $H = VP/S$  is combined from the CV (VP) and CV (S). In this case, if the input parameters are independent, the combined CV is calculated using the following equation:

$$CV_{combined} = \sqrt{\frac{\sum_{i=1}^n CV_i^2}{n}} \quad (\text{Eqn. 9})$$

where  $n$  is the number of parameters used in the multiplication/division and  $CV_i$  is the coefficient of variation in the  $i$ th input parameter.

## Benzene

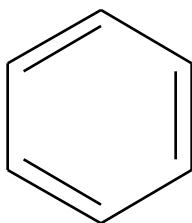
### Other Names

annulene, benzin, benzine, benzol, benzole, benzolene, bicarburet of hydrogen, carbon oil, CAS no. 71-43-2, coal naphtha, cyclohexatriene, DOT No. 1114, mineral naphtha, motor benzol, NCI-C55276, NIOSH No. CY 1400000 [Sax & Lewis (1989)]; nitration benzene, phene, phenyl hydride, polystream [WHO IARC (1982)]; pyrobenzol, pyrobenzole, RCRA Waste Number U109

### Background

Benzene was first recovered from light oil derived from coal-tar. Modern day commercial production of benzene is by catalytic reforming (dehydrogenation) of cycloparaffins. Other sources of benzene are the pyrolysis of gasoline; catalytic or thermal hydrodealkylation of toluene or xylenes and transalkylation of toluene. Benzene is also recovered from coal tar. Coking, liquefaction, and gasification of coal are all potential sources of benzene (Kirk-Othmer, 1984). Benzene is used primarily in the manufacture of other chemicals such as ethylbenzene, styrene, cumene, phenolic resins, ketones, adipic acid, caprolactam, nylon, and various dyes [Clayton and Clayton (1981)]. Benzene enters the atmosphere primarily from fugitive emissions and exhaust connected with its use in gasoline and as an industrial intermediate. It is volatile and mobile in soil, evaporates rapidly in water, and biodegrades slowly in aerobic soil. It does not bioconcentrate significantly in aquatic organisms or adsorb to soil but reacts with photochemically induced hydroxyl radicals in air.

### Formula



**MW: Molecular Weight**

The units used for molecular weight are grams/mole (g/mol).

*Estimated Values*

78.113	reported as a MW of 78.113 g/mol by Holden (1980) [also cited in Riddick (1986)]
78.11	reported as a MW of 78.11 g/mol by Kirk-Othmer (1984)
78.11	reported as a MW of 78.11 g/mol by Miller et al. (1985)
78.11	reported as a MW of 78.11 g/mol by Budavari et al. [Merck Index (1989)]
78.11	reported as a MW of 78.11 g/mol by Verscheuren (1983)

From the above 5 reported values above, we obtain the following statistics for the molecular weight of benzene:

Arithmetic mean (coefficient of variation):  
 MW = 78.11 ( $1.7 \times 10^{-5}$ ) g/mol

**K<sub>ow</sub>: Octanol-Water Partition Coefficient**

The units used for K<sub>ow</sub> are  $\frac{\text{mg/liter (octanol)}}{\text{mg/liter (water)}}$  and K<sub>ow</sub> is therefore unitless.

*Experimental Values*

182	reported at 18 °C as a log K <sub>ow</sub> of 2.26 by De Kock and Lord (1987) estimated using reverse phase-high performance liquid chromatography (RP-HPLC)
132	reported at 20 °C as a log K <sub>ow</sub> of 2.12 by Veith et al. (1980) using a shake flask-gas chromatogram (GC) method
135	reported at 20 °C as a log K <sub>ow</sub> of 2.13 by Freed et al. (1979) using a shake flask-gas/liquid chromatography (GLC) method
132	reported at 23 °C as a K <sub>ow</sub> of 132 by Banerjee et al. (1980) using a shake flask-liquid scintillation counting (LSC) method [Also cited in Mackay et al. (1992)]
170	reported at 23 °C as a log K <sub>ow</sub> of 2.23 by Harnish et al. (1983) estimated using a RP-HPLC method [Also cited in Mackay et al. (1992)]
103	reported at 25 °C as a ln K <sub>ow</sub> of 4.63 by Schantz & Martire (1987) estimated using a generator column-reverse phase liquid chromatography (GC-RPLC) [Also cited in Mackay et al. (1992)]
130	reported at 25 °C as a K <sub>ow</sub> of 130 by Karickhoff et al. (1979) using a shake flask-UV method

- 135 reported at 25 °C as a log  $K_{ow}$  of 2.13 by Veith et al. (1980) estimated using RPLC
- 135 reported at 25 °C as a log  $K_{ow}$  of 2.13 by Wasik (1981) estimated using a GC-high performance liquid chromatography (GC-HPLC) method
- 153 reported at 25 °C as a log  $K_{ow}$  of 2.186 by De Bruijn et al. (1989) using a slow stirring-GC method [Also cited in Mackay et al. (1992)]
- 158 reported at 25 °C as a log  $K_{ow}$  of 2.20 by Hammers et al. (1982) estimated using a RP-HPLC method [Also cited in Mackay et al. (1992)]
- 245 reported at 25 °C as a log  $K_{ow}$  of 2.39 by Veith et al. (1979) estimated using RP- HPLC

From the 12 measured values above we obtain the following statistics for the octanol-water partition coefficient of benzene at 25 °C:

Arithmetic mean (coefficient of variation):  
 $K_{ow} = 150 (0.24)$

Range:  $K_{ow} = 103$  to  $245$

### **$T_m$ : Melting Point**

The units used for melting point are kelvins (K).

#### *Experimental Values*

- 278.55 reported as an experimental MP of 5.4 °C by Gross and Saylor (1931)

From the measured value above, and the assumption that the CV is equal to the variation in this and "other values" recorded here, we obtain the following statistics for the melting point of benzene:

Arithmetic mean (coefficient of variation):  
 $T_m = 278.6 (2.5 \times 10^{-4}) \text{ K}$

#### *Other Values*

- 278.50 reported as 278.5 K by Miller et al. (1985)
- 278.65 reported as 5.5 °C by Budavari et al. [Merck Index (1989)]
- 278.65 reported as 5.5 °C by Verscheuren (1983)
- 278.66 reported as 5.51 °C by Sax and Lewis (1989)
- 278.683 reported as 5.533 °C by Kirk-Othmer (1985)
- 278.683 reported as 5.533 °C by Mackay (1992)



**VP: Vapor Pressure at Standard Temperatures**

The units used for vapor pressure are pascals (Pa).

*Experimental Values*

11906	interpolated to 25 °C from data by Stull (1947) using an Antoine equation and $-20 < T < 60.6$ °C
12636	reported at 298 K as 12636 Pa by Ambrose (1981) using an average of 3 measurements and an ebulliometric apparatus [Also cited in Mackay et al. (1992)]
12666	reported as $125 \times 10^{-3}$ atmospheres (atm) by Zwolinski and Wilhoit (1971)
12676	reported at 25 °C as 12.676 kPa by Willingham et al. (1945) estimated using an Antoine equation from pressured measurements $14.5 < T < 80.9$ °C [also cited in Boublik et al. (1984)]
12819	interpolated to 25 °C and corresponding to 12819 Pa from data by Gilman (1938) estimated using an Antoine equation and $36 < T < 75$ °C [also cited in Riddick (1986)]
13330	reported at 26 °C as 13.33 kPa by Kirk-Othmer (1979)

From the 6 measured values above, we obtain the following statistics for the vapor pressure of benzene at 25 °C:

Arithmetic mean (coefficient of variation):  
VP = 12700 (0.036) Pa

Range: 11906 to 13330 Pa

*Estimation Methods*

The following Antoine equations are derived from data in the temperature ranges reported below.

**Antoine Equation 1**

The following Antoine equation is derived from data in Stull (1947).

$$\log_{10} \text{VP} = 10.752389 - \frac{1989.6313}{273 + T \text{ (}^{\circ}\text{C)}}$$

using  $-20 < T < 60.6$  °C, yielding:

$$\text{VP} = 11906 \text{ Pa at } 298 \text{ K}$$

Antoine Equation 2

The following Antoine equation is derived from data in Willingham et al. (1945) [also in Boublik et al. (1984)]

$$\log_{10} VP = 6.1079 - \frac{1203.68}{219.904 + T (^{\circ}\text{C})}$$

using  $14.5 < T < 80.9$  °C, yielding:

$$VP = 12676 \text{ Pa at } 298 \text{ K}$$

Antoine Equation 3

The following Antoine equation is derived from data in Ambrose (1981) [also cited in Boublik et al. (1984)]

$$\log_{10} VP = 6.019 - \frac{1204.64}{273 + T (^{\circ}\text{C})}$$

using  $21 < T < 105$  °C, yielding:

$$VP = 12693 \text{ Pa at } 298 \text{ K}$$

**S: Solubility in Water**

The units used in the solubility values below are  $\frac{\text{mg}}{\text{liter (water)}}$  (mg/L).

*Experimental Values*

1402	reported at 25° as 0.16 ml/100 ml water by Booth & Everson (1948) using a residue-volume method
1650	reported at 25 °C as 1650 mg/L by Coutant & Keigley (1988) a using shake flask-GC method
1695	reported at 25 °C as 0.0217 mol/L by Keeley (1988) using a headspace analysis
1710	reported at 25 °C as 1710 ppm in water by Freed et al. (1979)
1718	reported at 25 °C as 0.022 mol/L by Taha (1966) [Also cited in Mackay et al. (1992)]
1731	reported at 26 °C as $3.99 \times 10^{-4}$ mol fraction by Franks et al. (1963) using a shake flask-UV method
1740	reported at 25 °C as 0.174 g/100 g solution by Arnold et al (1958) using a shake-flask UV method

1740	reported at 25 °C as 1740 mg/L by Price (1976) using a shake flask-GC method
1749	reported at 25 °C as a log 1/S of 1.65 mol/L by Veith et al. (1980) [also reported by Mackay et al. (1993)]
1750	reported at 25 °C as 22400 µM by Banerjee et al. (1980) [As cited in Horvath (1982)]
1755	reported at 25 °C as 1.775 mol/L by McDevit & Long (1952) using the Euler method
1765	reported at 25 °C as 1765 mg/L by Leinonen and Mackay (1975) using a shake flask-GC method
1780	reported at 25 °C as 1780 ppm by McAuliffe (1966) using a shake flask-GC method
1789	reported at 25 °C as 22.90 mol/m <sup>3</sup> by Miller et al. (1985)
1790	reported at 25 °C as 1.79 g/L saturated solution by Bohon & Claussen (1951) using a shake flask-UV method
1791	reported at 25 °C as 1791 mg/L by May et al. (1978) using a dynamic coupled column liquid chromatographic (DCCLC) method [also cited in Riddick (1986)]
1792	reported at 25 °C as $0.4129 \times 10^{-3}$ mole fraction by May et al. (1983) estimated using a generator column-HPLC method
1860	reported at 25 °C as 0.186 g/100 g water by Stearns et al. (1947) using a shake flask-turbidimetric method
1874	reported at 25 °C as a log S of -1.62 mol/L by Klevens (1950) using shake flask-UV
1878	reported at 25 °C as 0.1878 wt.% by Schwartz (1980) using a liquid phase elution chromatographic method
1906	reported at 25 °C as $24.4 \times 10^{-6}$ mol/g water by Vesala (1974) using a shake flask-UV method

#### *Unit Conversion*

Arithmetic mean (coefficient of variation) of benzene solubility

$$= 1755 (0.059) \text{ mg/L}$$

$$= 22 (0.059) \text{ mol/m}^3$$

From the 21 measured values above, we obtain the following statistics for the water solubility of benzene at 25 °C:

Arithmetic mean (coefficient of variation):  
 $S = 22 \text{ (0.059) mol/m}^3$

Range: 18 to 24.4 mol/m<sup>3</sup>

## H: Henry's Law Constant

The units used for Henry's Law constant are  $\frac{\text{Pascals-m}^3}{\text{mole}}$  (Pa-m<sup>3</sup>/mol).

### *Experimental Values*

758	reported at 20 °C as 0.306 unitless by Yurteri et al. (1987) using EPICS
458	reported at 25 °C as 0.00452 atm-m <sup>3</sup> /mole by Ashworth et al. (1988) using Equilibrium Partitioning in a Closed System (EPICS) [Also cited in Mackay et al. (1992)]
535	reported at 25 °C as 0.00528 atm-m <sup>3</sup> /mol by Ashworth et al. (1988) measured by EPICS
552	reported at 25 °C as 302 atm/mole fraction by Green & Frank (1979) based on concentration ratio/UV [Also cited in Mackay et al. (1992)]
562	reported at 25 °C as $5.55 \times 10^{-3}$ atm m <sup>3</sup> /mol by Mackay et al. (1979) using a batch stripping method [Also cited in Mackay et al. (1992)]
567	reported at 25 °C as $5.6 \times 10^{-3}$ atm-m <sup>3</sup> /mole by Warner et al. (1987) using a modified batch stripping apparatus (Mackay et al., 1979)
584	reported at 25 °C as $2.44 \times 10^{-5}$ torr/mole fraction by Keeley (1988) using a headspace analysis

From the 7 measured values above, we obtain the following statistics for Henry's law constant at 20-25 °C:

Arithmetic mean (coefficient of variation):  
 $H = 570 \text{ (0.16) Pa-m}^3/\text{mol}$

Range: 458 to 758 Pa-m<sup>3</sup>/mol

### *Estimation Method*

$$H = \frac{VP \text{ (Pa)}}{S \text{ (mol/m}^3\text{)}} = \frac{12700}{22} = 560 \text{ (0.049) Pa-m}^3/\text{mol}$$

**D<sub>air</sub>: Diffusion Coefficient in Pure Air**

The units used for the diffusion coefficient in pure air are  $\frac{\text{meters}^2}{\text{day}}$  (m<sup>2</sup>/d).

*Estimation Method*

Based on the Fuller et al. (1966) method described in Lyman et al. (1982), the estimated diffusion coefficient in air (m<sup>2</sup>/d) is given by:

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{(29 + M_x)/(29 \times M_x)}}{[2.7 + V_x^{1/3}]^2}$$

Molar volume ( $V_x$ ) can be estimated by the LeBas incremental method as described in Lyman et al. (1982) With a molar volume,  $V_x$ , of 96 cm<sup>3</sup>/mol, molecular weight ( $M_x$ ) of 78.11 g/mol, and a temperature equal to 298 K, the above expression gives:

$$D_{\text{air}} = 3.5 \times 10^{-5} T^{1.75} = 0.76 \text{ m}^2/\text{d}$$

The reported average absolute estimation error is 5 to 10% [Fuller et al. (1966)] and equivalent to the CV reported below.

Based on the estimated value and the estimation error reported above, we obtain the following statistics for the estimated air diffusion coefficient of benzene at 25 °C:

Arithmetic mean (coefficient of variation):

$$D_{\text{air}} = 0.76 (0.08) \text{ m}^2/\text{d}$$

**D<sub>water</sub>: Diffusion Coefficient in Pure Water**

The units used for the diffusion coefficient in pure water are  $\frac{\text{meters}^2}{\text{day}}$  (m<sup>2</sup>/d).

*Estimation Method*

Based on the Wilke and Chang (1955) method described in Reid et al. (1987) the diffusion coefficient in water (m<sup>2</sup>/d) is given by:

$$D_{\text{water}} = \frac{6.5 \times 10^{-7} \sqrt{f \times M_y} T}{h_y V_x^{0.6}}$$

Wilke and Chang (1955) recommend an association factor,  $f$ , of 2.6 when the solvent is water. The viscosity of water,  $\eta_y$ , is 0.89 cP at 25 °C. Molar volume ( $V_x$ ) can be estimated by the LeBas incremental method as described in Lyman et al. (1982). With a  $V_x$  equal to 96 cm<sup>3</sup>/mol, a temperature ( $T$ ) of 298 K, and  $M_y$  (MW of water) equal to 18 g/mol., this expression gives:

$$D_{\text{water}} = 3.2 \times 10^{-7} T = 9.6 \times 10^{-5} \text{ m}^2/\text{d at } 25 \text{ }^\circ\text{C}$$

Original data for this estimation, provided in Reid et al. (1987), can be used to determine the standard error of the estimator for this estimation method. From this data we calculate a CV of 0.25 from a 25% estimation error.

Based on the estimated value and the estimation error reported above, we obtain the following statistics for the estimated water diffusion coefficient of benzene at 25 °C:

Arithmetic mean (coefficient of variation):

$$D_{\text{water}} = 9.6 \times 10^{-5} (0.25) \text{ m}^2/\text{d}$$

### **$K_{oc}$ : Organic-Carbon Partition Coefficient**

The units used for  $K_{oc}$  are  $\frac{\text{mg/kg (organic carbon)}}{\text{mg/kg (water)}}$  and  $K_{oc}$  is therefore unitless.

#### *Experimental Values*

- 17 reported as an average  $K_{om}$  of 10.1 by Rutherford & Chiou (1992) using a peat and a muck soil (carbon fraction = 53%) and assuming  $K_{oc} = K_{om} \times 1.724$  [also cited in Mackay (1993)]
- 22 reported as a  $K_d$  of 0.57 by Lee et al. (1989) using an untreated A horizon Martlette soil (pH = 6.4,  $f_{oc} = 2.59$ )
- 22 reported at 24 °C as a  $K_{om}$  of 12.5 by Rutherford et al (1992) using peat and muck (57% carbon) and assuming  $K_{oc} = K_{om} \times 1.724$
- 26 reported as an average (sediment/water) log  $K_p$  of 0.02 by Vowles and Mantoura (1987) using a Tamar Estuary sediment ( $f_{oc} = 4.02\%$ ) for 1 hour
- 26 reported as an average  $K_d$  of 0.16 by Stuart et al. (1991) using batch competitive and batch non-competitive adsorption at 20 µg/L in an Aldelphia sandy loam ( $f_{oc} = 0.62\%$ )
- 31 reported at 20 °C as a log  $K_{om}$  of 1.26 by Chiou et al. (1983) using a Woodburn silt loam soil with 1.9% organic matter and assuming  $K_{oc} = K_{om} \times 1.724$

- 45 reported as an average  $K_{oc}$  of 45.1 by Seip et al. (1986) using 3 surface soils (pH = 4.2-7.4,  $f_{oc}$  = 0.2-3.7%) and 1.0 mg/L in a column elution study
- 46 reported as a (soil/water)  $K_p$  of 0.12 by Piwoni and Banerjee (1989) using soil ( $f_{oc}$  = .26% for 23 hrs at 10 to 300  $\mu\text{g/L}$ )
- 49 derived from an average log  $K_{oc}$  of 1.69 by Abdul et al. (1987) using a batch absorption method and sandy vadose-zone materials ( $f_{oc}$  = 1.05%)
- 54 reported at 20 °C as a  $K_d$  of 0.49 by Gan and Dupont (1989) using Skumpah and Kidman soils ( $f_{oc}$  = 0.9 ; pH = 8.0%) at 13 to 39 ppm benzene
- 55 reported as a  $K_p$  of 0.819 by Walton et al. (1992) using a Captina silt loam ( $f_{oc}$  = 1.49%; pH = 4.97) at 100 to 650  $\mu\text{g/g}$  benzene for 18 hours
- 64 reported as a  $K_p$  of 0.424 by Walton et al. (1992) using a McLaren sandy loam ( $f_{oc}$  = 0.66%; pH = 4.43) at 100 to 650  $\mu\text{g/g}$  benzene for 18 hours
- 79 reported as a log  $K_{oc}$  of 1.9 by Topp (1986) using soil ( $f_{oc}$  = 2.06%, pH = 6.4) for 1 week and  $^{14}\text{C}$  labelled benzene
- 83 reported at 25 °C as an average  $K_{oc}$  of 83 by Karickhoff et al. (1979) using 3 sediments ( $f_{oc}$  = 0.086 to 3.29%) and a shake-flask UV method
- 92 reported at 25 °C as a  $K_{oc}$  of 92 by Rogers et al. (1980) using radiolabelled benzene at 10, 100 and 1000 ppb for 136 hours with an Overton silty clay loam containing 2.6% organic carbon
- 100 reported at 25 °C as a  $K_{oc}$  of 100 by Rogers et al. (1980) using radiolabelled benzene at 10, 100 and 1000 ppb for 136 hours with a Hastings silty clay loam containing 1.8 % organic carbon
- 124 reported at 20 °C as a  $K_d$  of 0.62 by Gan and Dupont (1989) using a Kidman soil ( $f_{oc}$  = 0.5%; pH = 7.5%) at 13 to 39 ppm benzene

From the 17 measured values above, we obtain the following statistics for the organic carbon partition coefficient for benzene:

Arithmetic mean (coefficient of variation):  
 $K_{oc} = 55 (0.57)$

Range: 17 to 124

#### *Estimation Method*

Karickhoff (1981) has described empirical estimation methods for obtaining  $K_{oc}$  from  $K_{ow}$ . The most general of these is that  $K_{oc}$  is equal to 0.41 times  $K_{ow}$ .

$$K_{oc} = 0.41 \times K_{ow}$$

$$K_{ow} = 150$$

$$K_{oc} \text{ (est)} = 62 \text{ (1)}$$

The reported CV is based on data provided by Karickhoff (1981). This estimation error does not include uncertainty in the value of  $K_{ow}$ .

### **$K_{d_s}$ : Distribution Coefficient in Ground-Surface and Root-Zone Soil**

The units used for  $K_{d_s}$  are  $\frac{\text{mg/kg (dry surface and root-zone soil)}}{\text{mg/kg (water)}}$  and  $K_{d_s}$  is therefore unitless.

#### *Estimation Method*

This is a site specific parameter and depends on the fraction organic carbon in the surface and root-zone soil and on the value of  $K_{oc}$ .  $K_{d_s}$  is the product of the soil organic carbon partition coefficient ( $K_{oc}$ ) and the fraction organic carbon in the surface and root-zone soil ( $f_{oc_s}$ ) (Karickhoff, 1981).

$$K_{d_s} = K_{oc} \times f_{oc_s}$$

$$f_{oc_s} = \frac{\text{kg organic carbon (dry surface and root-zone soil)}}{\text{kg (soil)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in surface and root-zone soil.  $K_{d_s}$  is a site and soil-zone specific parameter depending on the fraction organic carbon in the surface and root-zone soil or:

$$K_{d_s} = K_{oc} \times f_{oc_s}$$

### **$K_{d_v}$ : Distribution Coefficient in Vadose-Zone Soil**

The units used for  $K_{d_v}$  are  $\frac{\text{mg/kg (dry vadose-zone soil)}}{\text{mg/kg (water)}}$  and  $K_{d_v}$  is therefore unitless.

#### *Estimation Method*

This is a site specific parameter and depends on the fraction organic carbon in the vadose-zone soil and on the value of  $K_{oc}$ .  $K_{d_v}$  is the product of the soil organic carbon partition coefficient ( $K_{oc}$ ) and the fraction organic carbon in the vadose-zone soil ( $f_{oc_v}$ ) (Karickhoff, 1981).



$$K_{d\_v} = K_{oc} \times f_{oc\_v}$$

$$f_{oc\_v} = \frac{\text{kg organic carbon (dry vadose-zone soil)}}{\text{kg (soil)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in vadose-zone soil.  $K_{d\_v}$  is a site and soil-zone specific parameter depending on the fraction organic carbon in the vadose-zone or:

$$K_{d\_v} = K_{oc} \times f_{oc\_v}$$

#### **$K_{d\_q}$ : Distribution Coefficient in the Ground-Water Zone**

The units used for  $K_{d\_q}$  are  $\frac{\text{mg/kg (dry aquifer material)}}{\text{mg/kg (water)}}$  and  $K_{d\_q}$  is therefore unitless.

##### *Estimation Method*

This is a site-specific parameter and depends on the fraction organic carbon in the ground-water zone and on the value of  $K_{oc}$ .  $K_{d\_q}$  is the product of the soil organic carbon partition coefficient ( $K_{oc}$ ) and the fraction organic carbon in the ground-water zone ( $f_{oc\_q}$ ) (Karickhoff, 1981).

$$K_{d\_q} = K_{oc} \times f_{oc\_q}$$

$$f_{oc\_q} = \frac{\text{kg organic carbon (dry aquifer material)}}{\text{kg (solid)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in the ground-water zone.  $K_{d\_q}$  is a site and soil-zone specific parameter depending on the fraction organic carbon in the ground-water zone or:

$$K_{d\_q} = K_{oc} \times f_{oc\_q}$$

**K<sub>d\_d</sub>: Distribution Coefficient in Sediment Particles**

The units used for K<sub>d\_d</sub> are  $\frac{\text{mg/kg (dry surface-water sediment)}}{\text{mg/kg (water)}}$  and K<sub>d\_d</sub> is therefore unitless.

*Estimation Method*

This is a site specific parameter and depends on the fraction organic carbon in the surface-water sediment and the value of K<sub>oc</sub>. K<sub>d\_d</sub> is the product of the soil organic carbon partition coefficient (K<sub>oc</sub>) and the fraction of organic carbon in surface-water sediment (f<sub>oc\_d</sub>) [Karickhoff, 1981].

$$K_{d_d} = K_{oc} \times f_{oc_d}$$

$$f_{oc_d} = \frac{\text{kg organic carbon (dry surface-water sediment)}}{\text{kg (soil)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in surface-water sediment particles. K<sub>d\_d</sub> is a site and soil-zone specific parameter depending on the fraction organic carbon in surface-water sediment or:

$$K_{d_d} = K_{oc} \times f_{oc_d}$$

**K<sub>ps</sub>: Partition Coefficient for Plant-Tissue (Above Ground Fresh Mass) Relative to Soil Concentration (Fresh Soil)**

The units used for K<sub>ps</sub> are  $\frac{\text{mg/kg (plant fresh mass [pFM])}}{\text{mg/kg (soil fresh mass [sFM])}}$  (ppm [pFM]/ppm [sFM])

*Experimental Values*

2.2 to 3.8 reported as a soil/plant BCF of 10 and 17 ppm plant dry mass (pDM)/ppm soil dry mass (sDM) by Topp et al. (1989) using Cress and Barley plants, respectively, after 12 days with <sup>14</sup>C benzene; we assume that soil is 90% dry mass and plants are 20% dry mass by weight

From the 2 values above, we obtain the following statistics for the plant-soil partition coefficient for benzene:

Arithmetic mean (coefficient of variation):  
K<sub>ps</sub> = 3.0 (0.38) ppm (pFM)/ppm (sFM)

*Estimation Method*

Based on a review of reported measurements of bioconcentration for 29 persistent organochlorines in plants, Travis and Arms (1988) have correlated plant-soil bioconcentration (on a dry-mass basis) in above-ground plant parts with octanol-water partition coefficients. This bioconcentration factor,  $B_v$ , on a dry-weight basis is expressed as:

$$\log B_v = 1.58 - 0.58 \log K_{ow} \pm 0.73 \text{ (n=29, } r^2=0.525)$$

We calculated the error term,  $\pm 0.73$ , from the mean square error of the estimator for this regression from the data provided by Travis and Arms (1988). When adjusted to a fresh-mass basis (assuming that the plant dry-mass fraction equals 0.2), this estimation equation gives the plant-soil partition coefficient,  $K_{ps}$ , expressing the ratio of contaminant concentration in mg/kg in above-ground plant fresh mass relative to contaminant concentration in mg/kg (dry soil) in the root-zone as:

$$K_{ps} = 7.7 K_{ow}^{-0.58} \text{ (CV = 4.0) ppm (plant FM)/ppm (soil DM)}$$

Expressing the ratio of contaminant concentration in mg/kg in above-ground plant fresh mass relative to contaminant concentration in mg/kg (fresh soil), and assuming fresh soil 10% by mass water in the root-zone soil, the  $K_{ps}$  estimation is:

$$K_{ps} \text{ (est)} = 7.0 K_{ow}^{-0.58}$$

$$K_{ow} = 150$$

$$K_{ps} \text{ (est)} = 0.39 \text{ ppm (plant FM)/ppm (soil FM)}$$

The estimation error reported above corresponds to a CV of 4.

 **$K_{pa}$ : Biotransfer Factors For Plant Leaves Relative to Contaminant Air Concentration**

The units used for  $K_{pa}$  are  $\frac{\text{mg/kg (plant fresh mass [pFM])}}{\text{mg/cubic meter of air (m}^3 \text{ [air])}} \text{ (m}^3 \text{ [a])/kg [pFM])}$

No reported measurements of  $K_{pa}$  for benzene are available in the current literature. An estimation method for this parameter is therefore applied.

*Estimation Method*

Based on the model of Riederer (1990) for foliar uptake of gas-phase contaminants ( $\text{mg}/\text{m}^3$ ) relative to contaminant concentration in plant leaves ( $\text{mg}/\text{kg}$  fresh mass), we estimate a steady-state plant-air coefficient as:

$$K_{\text{pa}} (\text{m}^3 [\text{a}]/\text{kg} [\text{pFM}]) = [0.5 + ((0.4 + 0.01 \times K_{\text{ow}})(RT/H))] \times 10^{-3} \text{ kg}/\text{m}^3$$

$$R = 8.313 \text{ Pa}\cdot\text{m}^3/\text{mol}\cdot\text{K}$$

$$T = 298 \text{ K}$$

$$H = 570 \text{ Pa}\cdot\text{m}^3/\text{mol}$$

$$K_{\text{ow}} = 150$$

$$K_{\text{pa}} (\text{est}) = 0.0087 \text{ m}^3 [\text{a}]/\text{kg} [\text{pFM}]$$

McKone (1993) has estimated that the CV associated with this partition estimation model is on the order of 14.

From the estimation method identified above, we obtain the following statistics for the partition coefficient in plant leaves relative to contaminant concentration in air for benzene:

Arithmetic mean (coefficient of variation):

$$K_{\text{pa}} = 0.0087 (14) \text{ m}^3 [\text{a}]/\text{kg} [\text{pFM}]$$

**BIOTRANSFER FACTORS FOR FOOD PRODUCTS**

The biotransfer factors  $B_t$ ,  $B_k$  and  $B_e$  are the steady-state contaminant concentrations in, respectively; fresh meat, milk, and eggs; divided by the animals daily contaminant intake, and are expressed in units of  $(\text{mg}/\text{kg})/(\text{mg}/\text{d})$  or  $\text{kg}/\text{d}$ .

 **$B_k$ : Steady-State Biotransfer Factors for Whole Milk Relative to Contaminant Intake by Cattle**

The units used for  $B_k$  are days/kg (milk) ( $\text{d}/\text{kg} [\text{milk}]$ ).

No reported measurements of  $B_k$  are available in the current literature. Estimation methods are therefore considered.

*Estimation Method 1*

Based on a review of biotransfer factors for 28 organic chemicals in milk Travis and Arms (1988) developed the following geometric-mean regressions for  $B_{k1}$  based on the octanol-water partition coefficient ( $K_{\text{ow}}$ ).

$$\log B_{k1} = \log K_{ow} - 8.1 \pm 0.84 \text{ (n = 28, } r^2 = 0.55)$$

Using the data provided by Travis and Arms (1988), we calculated the error term,  $\pm 0.84$ , from the mean square error of the estimator for this regression. This estimation error corresponds to a CV of 6. From the above expression and  $\log K_{ow}$  of 2.18, we obtain the following statistics for the  $B_{k1}$  of benzene:

$$B_{k1} \text{ (est)} = 1.2 \times 10^{-6} \text{ days/kg (milk)}$$

$$CV = 6$$

#### *Estimation Method 2*

The transfer of organic chemicals from animal feed to milk has also been expressed in terms of the fat-diet partition coefficient,  $K_{fd}$ , which is the steady-state ratio of contaminant concentration in animal fat (or lipid) to contaminant concentration in animal feed with units kg (feed)/kg (fat). Kenaga (1980) reviewed cattle-dietary feeding studies for 23 chemicals, and from these studies derived the following fat-diet equation relating  $K_{fd}$  to  $K_{ow}$ :

$$\log K_{fd} = 0.5 \log K_{ow} - 3.457 \pm 1 \text{ (n = 23, } r^2 = 0.62)$$

The estimation error in this expression,  $\pm 1$ , was calculated by Kenaga (1980). The above estimation error corresponds to a CV of 14. From the above expression with  $\log K_{ow}$  of 2.18, an assumed pasture intake by dairy cattle of 85 kg/d (McKone and Ryan, 1989), and an assumed fat content of 0.04 in milk; we obtain the following statistics for the  $B_{k2}$  of benzene:

$$B_{k2} \text{ (est)} = 2.0 \times 10^{-6} \text{ days/kg (milk)}$$

$$CV = 14$$

The estimation values reported above yield the arithmetic mean and CV reported below:

$$B_k \text{ (avg)} = 1.6 \times 10^{-6} \text{ days/kg (milk)}$$

$$CV = 11$$

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factor for milk relative to dietary contaminant intake by dairy cattle for benzene:

Arithmetic mean (coefficient of variation):

$$B_k = 1.6 \times 10^{-6} \text{ (11) days/kg (milk)}$$

#### **B<sub>t</sub>: Steady-State Biotransfer Factor for Meat Relative to Contaminant Intake by Cattle**

The units used for B<sub>t</sub> are days/kg (meat) (d/kg [meat]).

No reported measurements of cattle-meat biotransfer for benzene are available in the current literature. Estimation methods are therefore considered.

##### *Estimation Method 1*

Based on a review of biotransfer factors for 36 chemicals in meat, Travis and Arms (1988) developed the following geometric-mean regression for B<sub>t1</sub> based on the octanol-water partition coefficient, K<sub>ow</sub>.

$$\log B_{t1} = \log K_{ow} - 7.6 \pm 0.95 \text{ (n = 36, } r^2 = 0.67)$$

Using the data provided by Travis and Arms (1988), we calculated the error term,  $\pm 0.95$  from the mean square error of the estimator for this regression. This estimation errors corresponds to a CV of 11. From the above expression and a log K<sub>ow</sub> equal to 2.18, we obtain the following estimation:

$$B_{t1} \text{ (est)} = 3.8 \times 10^{-6} \text{ days/kg (meat)}$$

$$CV = 11$$

##### *Estimation Method 2*

The transfer of organic chemicals from animal feed to meat has also been expressed in terms of the fat-diet partition coefficient, K<sub>fd</sub>, which is the steady-state ratio of contaminant concentration in animal fat (or lipid) to contaminant concentration in animal feed with units kg (feed)/kg (fat). Kenaga (1980) reviewed cattle-dietary feeding studies for 23 chemicals, and from these studies derived the following fat-diet equation relating K<sub>fd</sub> to K<sub>ow</sub>:

$$\log K_{fd} = 0.5 \log K_{ow} - 3.457 \pm 1 \text{ (n = 23, } r^2 = 0.62)$$

The estimation error in this expression,  $\pm 1$ , was calculated by Kenaga (1980). The above estimation error corresponds to a CV of 14. From the above expression with  $\log K_{ow}$  equal to 2.18, an assumed pasture intake by beef cattle of 60 kg/d (McKone and Ryan, 1989), and an assumed fat content of 0.4 in meat; we obtain the following estimation:

$$B_{t2} \text{ (est)} = 2.9 \times 10^{-5} \text{ days/kg (meat)}$$

$$CV = 14$$

The estimation values reported above yield the arithmetic mean and CV reported below:

$$B_t \text{ (avg)} = 1.6 \times 10^{-5} \text{ days/kg (meat)}$$

$$CV = 13$$

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factor for meat relative to dietary contaminant intake by cattle for benzene:

Arithmetic mean (coefficient of variation):

$$B_t = 1.6 \times 10^{-5} \text{ (13) days/kg (meat)}$$

### **$B_e$ : Steady-State Biotransfer Factors for Eggs Relative to Dietary Contaminant Intake by Chickens**

The units used for  $B_e$  are days/kg (eggs) (d/kg [eggs]).

No reported measurements of egg-diet biotransfer for benzene are available in the current literature. An estimation method is therefore considered.

#### *Estimation Method*

Based on measurements of polychlorodibenzodioxins (PCDDs) and polychlorodibenzo-furans (PCDFs) concentrations in soil versus concentrations in egg-fat and adipose tissue of foraging chickens, Stephens et al. (1990) have shown that contaminant concentrations in animal fat correlate with soil concentrations. In addition, they found the fat-soil partition factor in chicken fat is roughly six times higher than the fat-soil partition factor in cattle. However, the fraction of total intake represented by soil in the chicken diet is higher than in the cattle diet. Based on these observation and what is discussed in the above  $B_k$  and  $B_t$  sections, we (a) assume that the fat-diet partition factor in chickens is similar to that in cattle, (b) use  $\log K_{fd} = \log K_{ow} - 4.9$  to estimate the  $K_{fd}$  for chickens, and (c) use the fat content of eggs (0.08) and feed intake of chickens (0.12 kg/d [fresh mass]) to

obtain the following estimate of a biotransfer factor,  $B_e$ , from chicken diet to eggs with units d/kg (eggs):

$$\log B_e = \log K_{ow} - 5.1$$

$$\log K_{ow} = 2.18$$

$$B_e = 0.0012 \text{ d/kg (eggs)}$$

We estimate the CV in this expression is 14.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factors for egg concentration relative to dietary contaminant intake by chickens for benzene:

Arithmetic mean (coefficient of variation):

$$B_e = 0.0012 (14) \text{ days/kg (eggs)}$$

**$B_{bmk}$ : Biotransfer Factor for Human Breast Milk Relative to Dietary Contaminant Intake by the Mother**

The units used for  $B_{bmk}$  are days/kg (mothers milk) (d/kg [mothers milk]).

No experimental results quantifying  $B_{bmk}$  are available in the current literature. an estimation method (Smith, 1987), is therefore applied.

*Estimation Method*

$$B_{bmk} = 2 \times 10^{-7} K_{ow}$$

$$K_{ow} = 150$$

$$B_{bmk} = 3.0 \times 10^{-5} \text{ days/kg (mothers milk)}$$

The CV of the above method is approximately 10.



Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated biotransfer factor for human breast milk concentration relative to dietary contaminant intake by the mother for benzene:

$$\text{Arithmetic mean (coefficient of variation):}$$

$$B_{\text{bm}} = 3.0 \times 10^{-5} \text{ (10) days/kg (mothers milk)}$$

### BCF: Bioconcentration Factors for Fish Relative to Water Concentration

The units used for BCF (fish/water) are  $\frac{\text{mg/kg (fish)}}{\text{mg/liter (water)}}$ , and BCF is therefore unitless.

#### *Experimental Values:*

- 4 reported as a log BCF (fish/water) of 0.63 by Ogata et al. (1984) using goldfish at 1 ppm benzene
- 6.1 reported as a fish BCF of 6.1 by Korn et al. (1976) using  $22.7 \times 10^{-6}$  L benzene/kg (Northern anchovie muscle tissue) and  $3.7 \times 10^{-6}$  L benzene/L water in a static test for 2 days in seawater
- 10 reported as a fish BCF of 10 by Freitag (1987) using Golden Ide (*Idus idus melanotus*) for 3 days

From the 3 measured values reported above, we obtain the following statistics for BCF in fish relative to contaminant concentration in water for benzene:

$$\text{Arithmetic mean (coefficient of variation):}$$

$$\text{BCF (fish/water)} = 6.8 \text{ (0.43)}$$

Range: 4 to 10

#### *Estimation Method*

For fish, the BCF is taken as the ratio of concentration of a xenobiotic substance in fish flesh (or lipids) to the contaminant's concentration in water (Mackay, 1982). The BCF for neutral organic compounds can be estimated from regression equations based on selected physicochemical properties, particularly a compound's  $K_{\text{ow}}$  or aqueous solubility. Mackay (1982) recommends:

$$\text{BCF} = 0.048 K_{\text{ow}}$$

$$K_{\text{ow}} = 150$$

$$\text{BCF (est)} = 7.8$$

$$\text{CV} = 0.6$$

The reported GSD is 1.8 which corresponds to an estimation error of 0.6.

**K<sub>p\_w</sub>: Human Skin Permeability Coefficient Relative to Contaminant Concentration in Water**

The units used for K<sub>p\_w</sub> are centimeters/hour (cm/hr).

*Experimental Values*

- 0.11 reported at 30 °C as a permeability constant of 0.111 cm/hr. by Blank and McAuliffe (1984) using human skin in vitro, 2 µm/ml. conc., and a 40 µm thickness
- 0.26 reported at 30 °C as a benzene rate of 99 µg cm<sup>2</sup>/hr by Loden (1986a) using Teflon flow-through diffusion cells, 1920 µg adsorbed, and full thickness (0.2 cm) human skin (*in vitro*) for 13.5 hours

From the 2 measured values reported above, we obtain the following statistics for the human skin permeability coefficient for benzene:

Arithmetic mean (coefficient of variation):

$$K_{p_w} = 0.19 (0.57) \text{ cm/hr}$$

Range: 0.11 to 0.26 cm/hr

*Estimation Method*

Because dermal transfer is considered a nonsteady-state event, diffusion models require input parameters which are difficult to measure, such as the stratum corneum diffusion coefficient (D<sub>sc</sub>) [Flynn and Amidon, 1991]. Estimation of aqueous biotransfer of benzene is calculated with the following equation based on the estimation method of McKone and Howd (1992).

$$K_{p_w} = MW^{-0.6} 0.33 + \frac{0.0025}{2.4 \times 10^{-6} + 3 \times 10^{-5} K_{ow}^{0.8}}^{-1}$$

$$K_{ow} = 150$$

$$MW = 78.11 \text{ g/mol}$$

$$K_{p_w} = 0.040 \text{ cm/hr}$$

who report a coefficient of variation equal to 2.4

**K<sub>m</sub>: Partition Coefficient for Human Skin Relative to Contaminant Concentration in Water or Soil**

The units used for K<sub>m</sub> are  $\frac{\text{mg/kg (skin)}}{\text{mg/liter (water)}} (\text{ppm [skin]}/\text{ppm [water]})$ .

*Experimental Values*

- 0.50      calculated from data by Morgan et al. (1991) using aqueous absorption at 2/3 saturation in 24 hours; 0.26 ml absorption of 1164 µg/ml solution into 3.1 cm<sup>2</sup> of male rat skin
- 30        reported at 31 °C as a stratum corneum water partition coefficient of 30 by Blank and McAuliffe (1985) using human skin in vitro, 2 µg/ml conc., and a 40 µg thickness

From the 2 measured values\* reported above, we obtain the following statistics for the partition coefficient for human skin relative to contaminant concentration in water or soil for benzene:

Arithmetic mean (coefficient of variation):  
K<sub>m</sub> = 15 (1.4) ppm (skin)/ppm (water)

Range: 0.50 to 30 ppm (skin)/ppm (water)

*Estimation Method*

Experimental values quantifying dermal transfer of benzene in water, or for water in a soil matrix, may depend on pH, particle size and organic carbon content (Flynn and Amidon, 1991). An estimation method based on McKone and Howd (1992) is therefore used here.

$$K_m = 0.64 + (0.25 K_{ow}^{0.8})$$

$$K_{ow} = 150$$

$$K_m = 15 \text{ ppm (skin)}/\text{ppm (water)}$$

The reported geometric standard deviation of 1.3 in this estimation method corresponds to a CV of 0.27.

**T<sub>half\_a</sub>: Reaction Half-Life in Air**

The units used for T<sub>half\_a</sub> are days.

- 0.11 to 0.29      reported at 25 °C as a hydroxyl radical reaction rate constant (K<sub>OH</sub>) of 2.8 to 7.0 × 10<sup>-11</sup> cm<sup>3</sup>/molecule-sec by Lorenz and Zellner (1983) using pressures of 1.5 to 42 mbar; assuming an average atmospheric [OH] of 1 × 10<sup>6</sup> molecules/cm<sup>3</sup>

- 5.0 reported at 25 °C as a  $K_{OH}$  of  $1.59 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Davis et al. (1975) using 100 torr of helium; assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 5.7 reported at 27 °C as a  $K_{OH}$  of  $1.4 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Singh et al. (1981) using field air sample collections; assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 6.4 reported at 23 °C as a  $K_{OH}$  of  $1.26 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Edney (1986) assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 6.4 reported at 25 °C as a  $K_{OH}$  of  $1.25 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Tully et al. (1981) using 100 torr [He]; assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 6.5 reported at 298 K as a  $K_{OH}$  of  $1.24 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Hansen et al. (1975) using a flash photolysis resonance fluorescence technique at 50 to 600 torr [Ar],  $1 \times 10^{11}$  molecules benzene/cm<sup>3</sup>; assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 6.6 reported at 25 °C as a  $K_{OH}$  of  $1.21 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Tully et al. (1981) using 100 torr [Ar]; assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 6.7 reported at 298 K as a  $K_{OH}$  of  $1.2 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Perry et al. (1977) using a flash photolysis resonance fluorescence technique at 100 torr [Ar]; assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 8.0 reported at 23 °C as a  $K_{OH}$  of  $1.0 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Rinke and Zetzsch (1984) assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 9.1 reported at 22 °C as a  $K_{OH}$  of  $8.8 \times 10^{-13}$  cm<sup>3</sup>/molecule-sec by Wahner and Zetzsch (1983) using 133 mbar [AR]; assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>
- 10 reported at 27 °C as a  $K_{OH}$  of  $0.8 \times 10^{-12}$  cm<sup>3</sup>/molecule-sec by Cox et al. (1980) assuming an average atmospheric [OH] of  $1 \times 10^6$  molecules/cm<sup>3</sup>

From the 12 experimental values reported above, we obtain the following statistics on the reaction half-life for benzene in air at 25 °C:

Arithmetic mean (coefficient of variation):

$$T_{half\_a} = 5.9 (0.51) \text{ days}$$

Range: 0.11 to 10 days

**T<sub>half\_g</sub>: Reaction Half-Life in Ground-Surface Soil**

The units used for T<sub>half\_g</sub> are days.

*Reported Values*

30 to 121 reported at 25 °C as an aerobic degradation rate in soil of 14.85 and 47.08% by Watwood et al. (1991) using a Sandia and a Bosque unsaturated calcareous soils from New Mexico, 100 ppb, and <sup>14</sup>C labelled benzene for 4 weeks; assuming first-order kinetics

From the 2 values above, and the assumption that the actual range of values may be a factor of 5 higher of lower than this range, we obtain the following statistics for the reaction half-life for benzene in surface soil:

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_g} = 190 (1.5) \text{ days}$$

Range: 6.1 to 603 days

**T<sub>half\_s</sub>: Reaction Half-Life in Root-Zone Soil**

The units used for T<sub>half\_s</sub> are days.

*Reported Values*

30 to 121 reported at 25 °C as an aerobic degradation rate in soil of 14.85 and 47.08% by Watwood et al. (1991) using a Sandia and a Bosque unsaturated calcareous soils from New Mexico, 100 ppb, and <sup>14</sup>C labelled benzene for 4 weeks; assuming first-order kinetics

From the 2 values above, and the assumption that the actual range of values may be a factor of 5 higher of lower than this range, we obtain the following statistics for the reaction half-life for benzene in root-zone soil:

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_s} = 190 (1.5) \text{ days}$$

Range: 6.1 to 603 days

**T<sub>half\_v</sub>: Reaction Half-Life in Vadose-Zone Soil**

The units used for T<sub>half\_v</sub> are days.

*Experimental Values*

30 to 121	reported at 25 °C as an aerobic degradation rate in soil of 14.85 and 47.08% by Watwood et al. (1991) using a Sandia and a Bosque unsaturated calcareous soils from New Mexico, 100 ppb, and <sup>14</sup> C labelled benzene for 4 weeks; assuming first-order kinetics
154	reported at 17 °C as a half-life corresponding to 154 days by Wilson et al. (1986) using aquifer samples (pH = 7.3; organic carbon = 344 mg/L) incubated in a dark methanogenic microcosm for 120 weeks and assuming first order kinetics
108 to 789	reported at 25 °C as an anaerobic degradation rate in soil of 2.43 and 16.49% by Watwood et al. (1991) using a Sandia and a Bosque unsaturated calcareous soils from New Mexico, 100 ppb, and <sup>14</sup> C labelled benzene for 4 weeks; assuming first-order kinetics

From the 5 values above, we obtain the following statistics for the reaction half-life for benzene in vadose-zone soil at 25 °C:

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_v} = 240 (1.3) \text{ days}$$

Range: 30 to 789 days

**T<sub>half\_q</sub>: Reaction Half-Life in Groundwater**

The units used for T<sub>half\_q</sub> are days.

*Experimental Values*

50 to 116	reported 10 °C as a zero order degradation rate of -30 and 58 mg/d by Barker et al. (1987) using a 2.6 to mg/L in laboratory and field experiments with material from a sandy aquifer also containing xylene and toluene
154	reported at 17 °C as a half-life corresponding to 154 days by Wilson et al. (1986) using aquifer samples (pH = 7.3; organic carbon = 344 mg/L) incubated in a dark methanogenic microcosm for 120 weeks and assuming first order kinetics
108 to 789	reported at 25 °C as an anaerobic degradation rate in soil of 2.43 and 16.49% by Watwood et al. (1991) using a Sandia and a Bosque unsaturated calcareous soils from New Mexico, 100 ppb, and <sup>14</sup> C labelled benzene for 4 weeks; assuming first-order kinetics

From the 5 values above, we obtain the following statistics for the reaction half-life for benzene in groundwater:

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_q} = 240 (1.3) \text{ days}$$

Range: 50 to 789 days

### **$T_{\text{half}_w}$ : Reaction Half-Life in Surface Water**

The units used for  $T_{\text{half}_w}$  are days.

#### *Experimental Values*

- |         |  |
|---------|--|
| 5 to 16 | reported as a half-life of 5 to 16 days by Van der Linden (1978) using an aqueous aerobic biodegradation dieaway test in seawater [This study is also cited in Mackay et al. (1992)]   |
| 6       | reported at 22 °C as an aqueous aerobic biodegradation half-life of 6 days by Lee and Ryan (1979) using <sup>14</sup> C benzene in for 4 days in an estuarine river water and sediment mixture [This study is also cited Mackay et al. (1992)] |
| 7       | reported at 25 °C as a half-life in water of 7 days by Tabak et al. (1981) using domestic wastewater conditions in a static-culture flask-screening procedure for 28 days in the dark  |
| 16      | reported at 21 °C as a half-life of 16 days by Vaishnav and Babeu (1987) using an aqueous aerobic biodegradation dieaway test from water found in the Lester River, MN (pH = 7.76); assuming first order kinetics                              |
| 16.9    | reported at 20 °C as a photolysis half-life in water of 16.9 days by Hustert et al. (1981) using 1810 ppm benzene and assuming first-order kinetics  |

From the 6 values above, we obtain the following statistics for the half-life for benzene in surface water at 25 °C:

Arithmetic mean (coefficient of variation):

$$T_{\text{half}_w} = 11 (0.51) \text{ days}$$

Range: 5 to 16.9 days

**T<sub>half\_d</sub>: Reaction Half-Life in Surface Water Sediment**

The units used for T<sub>half\_d</sub> are days.

*Experimental Values*

- |            |   |
|------------|---|
| 6          | reported at 22 °C as an aqueous aerobic biodegradation half-life of 6 days by Lee and Ryan (1979) using <sup>14</sup> C benzene in for 4 days in an estuarine river water and sediment mixture [This study is also cited Mackay et al. (1992)]                            |
| 60         | reported at 10 and 20 °C as an methanogenic degradation half-life of 60 days by van Beelen and van Keulen (1990) using sediment (7.4 pH, 5% organic carbon) from the Merwede R. for 63 days at 1 to 100 µg/L and <sup>14</sup> C benzene                                  |
| 154        | reported at 17 °C as a half-life corresponding to 154 days by Wilson et al. (1986) using aquifer samples (pH = 7.3; organic carbon = 344 mg/L) incubated in a dark methanogenic microcosm for 120 weeks and assuming first order kinetics                                 |
| 108 to 789 | reported at 25 °C as an anaerobic degradation rate in soil of 2.43 and 16.49% by Watwood et al. (1991) using a Sandia and a Bosque unsaturated calcareous soils from New Mexico, 100 ppb, and <sup>14</sup> C labelled benzene for 4 weeks; assuming first-order kinetics |

From the 5 values above, we obtain the following statistics for the half-life of benzene in sediment at 25 °C:

Arithmetic mean (coefficient of variation):  
T<sub>half\_d</sub> = 220 (1.4) days

Range: 6 to 789 days

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